EXAFS Measurement of Bond-length Strain in Thin Gd_2O_3 Films on GaAs(001)

The extended x-ray absorption fine structure (EXAFS) technique was used to measure the bond length in a 2.3 nm thin Gd_2O_3 film grown epitaxially on GaAs(001). The Gd-O bond length is determined to be 0.2390 ± 0.0013 nm, which is a +2.7 ± 0.6 % bond-length strain relative to that in bulk Gd_2O_3 powder. We develop a model for the thin film relating macroscopic strain to microscopic atomic displacements.

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The long search for a stable, passivating surface oxide for GaAs possibly has ended with the development of Gd_2O_3 films. These epitaxially grown films are single crystal with a low number of defects and interfacial states, and they successfully have been used to fabricate metal-oxide-semiconductor structures on GaAs. We studied a 2.3 nm thin Gd_2O_3 film grown epitaxially on the GaAs(001) substrate at Bell Laboratories, Lucent Technologies.

EXAFS experiments were performed at NIST beamline X23-A2 at the National Synchrotron Light Source. The Gd Lα fluorescence yield around the Gd L_{III} edge (hν = 7243 eV) was monitored using a single-element SiLi detector. EXAFS data were recorded with the sample surface normal **n** either parallel (**ε** ∥ **n**) or perpendicular (**ε** ⊥ **n**) to the polarization vector **ε** of the synchrotron radiation. In addition, EXAFS data from a pure Gd_2O_3 powder were collected in transmission, to determine the EXAFS phase and amplitude standards for the Gd-O bond length.

Figure 1 shows the k^2-weighted Gd L_{III} edge EXAFS from the Gd_2O_3 powder. Also shown are the EXAFS from the Gd_2O_3 epitaxial film recorded in the two polarizations. The frequency of the EXAFS oscillations and, therefore, the Gd-O bond length r in the film is increased significantly relative to the powder. The best fits produce r = 0.2391 ± 0.0017 nm for **ε** ∥ **n** and r = 0.2389 ± 0.0019 nm for **ε** ⊥ **n**, so together we determine an average Gd-O bond length r = 0.2390 ± 0.0013 nm. This is a +0.0063 ± 0.0013 nm or +2.7 ± 0.6 % increase relative to the 0.2327 nm bond length in bulk Gd_2O_3 .

In addition, the data from the two polarizations are identical within the noise throughout the entire k range. This indicates that the first and second shell local structures are similar along the [110] and [-110] directions of the strained Gd_2O_3 film; therefore, the strains along [110] and [-110] are equal, as suggested by the crystal symmetry of Gd_2O_3 (see Figure 2).

We developed a simple model for the strained film, with a unique Poisson distortion that matches the [001] and [-110] axes of Gd_2O_3 with the [110] and [1-10] axes of the GaAs(001) surface. This model assumes that the microscopic displacements of the atoms are proportional to the macroscopic changes in the lattice constants. Using this model, the measured bond-length increase of the film determined by EXAFS agrees well with the perpendicular lattice distortion of the film determined by diffraction.

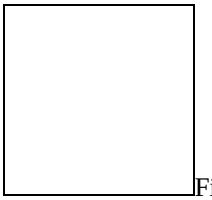

Figure 1. k^2-weighted Gd L_{III} edge EXAFS data from the bulk standard Gd_2O_3 powder (top). Also shown are the EXAFS from the thin Gd_2O_3 film on GaAs(001), with the X-ray polarization vector aligned parallel (middle, **ε** ∥ **n**) and perpendicular (bottom, **ε** ⊥ **n**) to the GaAs(001) surface normal. Lines are best fits to the first-shell component.

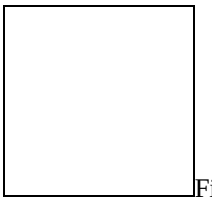

Figure 2. Local environment of the Gd atoms (right). Each Gd atom is surrounded by a distorted octahedron of 6 O atoms. The Gd-O bonds form "diamond" chains along the [110] and [-110] directions of the unit cell (left).

Contributors and Collaborators

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